Sundance: A High-Level Toolkit for Efficient, Parallel PDE Simulation and Optimization

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High-performance algorithms for PDE-constrained optimization[1] often require application of operators and solution of systems of equations that are different from those used in a single solution of the PDE; consequently, implementation of a fast gradient-based optimization algorithm often entails costs for modification to the PDE solver. A software tool to enable rapid development of parallel codes for large-scale, complex PDEs on realistic problems would be a useful aid to the development and application of fast PDE-constrained optimization algorithms. As part of Sandia's research efforts in PDE-constrained optimization, we are developing Sundance, an environment in which a parallel PDE system is accessed via a high-level problem description, using abstract concepts such as functions, operators, and regions. With this high-level problem description, it is possible to specify a variational formulation of a PDE and its discretization method in a small amount of user-level code. It is then straightforward to obtain operators such as Jacobians and Hessians for use in optimization algorithms.

While high-level software facilitates rapid development, it is a challenge to make high-level software efficient. In this presentation we will describe the methods by which Sundance realizes efficient matrix and vector assembly from a high-level problem specification via a hybrid symbolic-automatic differentiation algorithm. We will then show examples of the use of Sundance to implement highly efficient algorithms for optimization of systems described by PDE models.

References

[1] B. van Bloemen Waanders, R. Bartlett, K. Long, P. Boggs, and A. Salinger, "Large-Scale Nonlinear Programming for PDE-Constrained Optimization" Sandia National Laboratories Technical Report, SAND 2002-3198, 2002.